Fast, High-Order Solution of Surface Scattering Problems

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Introduction. We present a new algorithm for the numerical solution of problems of acoustic scattering by surfaces in three-dimensional space. This algorithm evaluates scattered fields through fast, high-order solution of the corresponding boundary integral equation. The high-order accuracy of our solver is achieved through use of *partitions of unity* together with *analytical* resolution of kernel singularities. The acceleration, in turn, results from use of a novel approach which, based on high-order *"two-face" equivalent source* approximations, reduces the evaluation of far interactions to evaluation of 3-D FFTs. This approach is faster, substantially more accurate, and it runs on dramatically lower memories than other FFT and k-space methods. The present algorithm computes one matrix-vector multiply in $\mathcal{O}\left(N^{6/5}\log N\right)$ to $\mathcal{O}(N^{4/3}\log N)$ operations, where N is the number of surface discretization points. The latter estimate applies to smooth surfaces, for which our high order algorithm provides accurate solutions with small values of N; the former, more favorable count is valid for highly complex surfaces requiring significant amounts of subwavelength sampling. Further, our approach exhibits super-algebraic convergence, it can be applied to smooth and non-smooth scatterers, and, unlike other accelerated schemes it does not suffer from accuracy breakdowns of any kind (compare [6, 10] and [8, p. 576]). In what follows we introduce the main algorithmic components in our approach, and we demonstrate its performance with a variety of numerical results. In particular, we show that the present algorithm can evaluate accurately in a personal computer scattering from bodies of acoustical sizes of several hundreds.

Mathematical Formulation. We consider a problem of acoustic scattering by a sound-soft obstacle. This problem, governed by the Helmholtz equation, can be treated using the acoustic single- and double- layer potentials (see e.g. [7])

$$(S\varphi)(\mathbf{r}') = \int_{\partial D} \Phi(\mathbf{r}',\mathbf{r})\varphi(\mathbf{r})ds(\mathbf{r}) \quad \text{and} \quad (K\varphi)(\mathbf{r}') = \int_{\partial D} \frac{\partial\Phi(\mathbf{r}',\mathbf{r})}{\partial\nu(\mathbf{r})}\varphi(\mathbf{r})ds(\mathbf{r}). \quad (1)$$

Here $\Phi(\mathbf{r}',\mathbf{r}) = e^{ik|\mathbf{r}'-\mathbf{r}|}/4\pi\,|\mathbf{r}'-\mathbf{r}|$ is the Green function for the Helmholtz equation, and $\nu(\mathbf{r})$ is the external normal to the surface ∂D at point $\mathbf{r}$. Explicitly, given the values of the incoming wave $\psi^i(\mathbf{r})$ on ∂D, the scattered field can be obtained easily once the integral equation for the unknown density $\varphi(\mathbf{r})$

$$\frac{1}{2}\varphi(\mathbf{r}) + (K\varphi)(\mathbf{r}) - i\eta\,(S\varphi)(\mathbf{r}) = \psi^i(\mathbf{r}), \qquad \mathbf{r}\in\partial D \quad (2)$$

has been solved. Naturally, the possibility of producing fast and accurate solutions for our problems hinges on our ability to evaluate the integrals (1) accurately

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and efficiently. In attempting to develop such accurate and efficient integrators one faces two main problems, namely, accurate evaluation of the singular *adjacent interactions* — without undue compromise of speed — and fast evaluation of the voluminous number of *nonadjacent interactions* — without compromise in accuracy. In what follows we present a solution to these problems.

Partitions of unity. In order to deal with topological characteristics of closed surfaces which are given in terms of local parametrizations we utilize partitions of unity. In detail, we use a covering of the surface ∂D by a number K of overlapping two-dimensional patches $\mathcal{P}^j, j = 1, \cdots, K$, (called local charts in differential geometry). The patches $\mathcal{P}^j$ are then smoothly mapped to coordinate sets $\mathcal{H}^j$ in two-dimensional space, where actual integrations are performed. Further, we utilize a partition of unity subordinated to this covering of ∂D, i.e. we introduce a set of non-negative smooth functions $\{w^j, j = 1, \ldots, K\}$, such that (i) w^j is defined, smooth and non-negative in ∂D, and it vanishes outside $\mathcal{P}^j$, and (ii) $\sum_{j=1}^{K} w^j = 1$ throughout ∂D. This allows us to reduce the problem of integration of the density $\varphi(\mathbf{r})$ over the surface to a calculation of integrals of smooth functions φ^j compactly supported in the planar sets $\mathcal{H}^j$.

Adjacent integration. Substantial difficulties in the high-order evaluation of *adjacent interactions* are caused by the singular nature of the integral kernels. While, certainly, the well-known strategy of "singularity subtraction" gives rise to bounded integrands, integration of such bounded functions by means of classical high-order methods does not exhibit high-order accuracy — since the subsequent derivatives of the integrand are themselves unbounded. The new basic high-order integrator we present is based on analytical resolution of singularities. The resolution is achieved by integration in polar coordinates centered around each singular point. The Jacobian of the corresponding change of variables has the effect of cancelling the singularity, so that high order integration in the both radial and angular directions can be performed using the trapezoidal rule. Since the corresponding radial quadrature points do not lie on the Cartesian grid, a high-order, fast interpolation technique has been developed for evaluation of the necessary function values at the radial integrations points. Efficiency is of utmost importance here, since we use one such polar coordinate transformation *at each target point.* Our high order integrator exhibits super-algebraic convergence for smooth and non-smooth scattering surfaces [1–3].

Non-adjacent integration and acceleration. Our accelerator is closely related to two of the most advanced FFT methods developed recently [4, 9]. An important common element between these two methods and our technique is a concept of equivalent (or auxiliary) sources, located on a subset of a 3-D Cartesian grid. In all three cases, the intensities of these sources are chosen to approximate the field radiated by the scatterer, which allows for fast computation of the "non-adjacent interactions" through the use of 3-D FFTs. Surface problems like the ones we consider are treated in [4, 9] by means of equivalent sources located in a *volumetric* grid — in such a way that equivalent sources with non-zero intensities occupy *all Cartesian nodes adjacent to the scatterer.* Since the spacing of this Cartesian grid cannot be coarsened beyond some threshold for surface

problems such a scheme requires a $\mathcal{O}(N^{3/2})$ FFT. Therefore, previous FFT surface scattering solvers require $\mathcal{O}(N^{3/2})$ units of RAM and they run in $\mathcal{O}\left(N^{3/2}\log N\right)$ operations. Our algorithm, in contrast, subdivides the volume occupied by the scatterer into a number of (relatively large) cubic cells, and it places equivalent sources *on the faces* of those cells. As we have shown, such a design reduces significantly the sizes of the required FFTs — to as little as $\mathcal{O}\left(N^{6/5}\right)$ to $\mathcal{O}\left(N^{4/3}\right)$ points — with proportional improvement in storage requirements and operation count. Further, it results in super-algebraic convergence of the equivalent source approximations *as the size of the scatterer is increased.*

Resolution of singularities To obtain resolution of the singular integrands around the ogive's conical singularities, for example, a combination of two changes of variables were used: a polar change of variables similar to that described in the section "Adjacent integration" above, followed by a polynomial change of variables which regularizes the Hölder-type singularity of the underlying density; see [3] for details.

Numerical Results. We present results for two well known and widely used test geometries: large ellipsoids and ogives. Solutions of the linear systems arising from discretization of equations (2) were obtained in all cases by means of a version of the iterative solver GMRES. In all cases we used the value $\gamma = \max\{3, A/\lambda\}$ for the coupling constant in equation (2) — where A is the diameter of the scatterer. We have found that this value of γ leads to a substantially reduced number of GMRES iterations. All computations were performed on a 400 MHz Pentium II processor and with 1Gb of RAM. In the following tables we used boundary conditions as given by a unit source located inside the ogive for which the exact solution is known: it equals the field radiated by the source. Convergence studies for plane-wave boundary conditions showed errors consistent with those displayed in these tables. The symbols ε_2 and ε_∞ denote the far field errors in the relative mean-square norm and the absolute maximum norm, respectively

Size	# It	T/it	RAM	Unknowns	ε_∞	ε_2
$80\lambda \times 20\lambda \times 20\lambda$	15	5h 22m	$600M$	691206	$1.4{\cdot}10^{-4}$	$2.9{\cdot}10^{-5}$
$100\lambda \times 25\lambda \times 25\lambda$	15	5h 29m	$600M$	691206	$1.1{\cdot}10^{-3}$	$2.4{\cdot}10^{-4}$

Table 1: Scattering from large ellipsoids; point source inside the body.

Table 1 presents results for problems of scattering by very large ellipsoids; note the excellent accuracies provided by the algorithm in competitive running times. Table 2 displays a set of results obtained for scattering from a singular surface: the ogive depicted in Figure 1, for acoustical sizes (distances between tips) equal to 1λ, 10λ and 20λ. For the larger sizes we used the accelerator described above; note the substantial improvements in computing times resulting from the acceleration algorithm.

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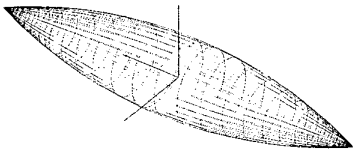

Figure 1: Ogive geometry presented in reference [11].

Type	Size	Unknowns	Iterations	Time/It.	ε_∞	ε_2
Non Accelerated	1λ	1568	20	69s	2.5×10^{-3}	$1.4 \cdot 10^{-3}$
Non Accelerated	1λ	6336	17	12m 45s	3.8×10^{-5}	$2.2 \cdot 10^{-5}$
Non Accelerated	1λ	25472	17	3h 27m	9.8×10^{-7}	$4.8 \cdot 10^{-7}$
Accelerated	10λ	34112	13	26m	3.8×10^{-4}	$2.1 \cdot 10^{-4}$
Accelerated	20λ	34112	14	14m	6.0×10^{-3}	$2.4 \cdot 10^{-3}$
Accelerated	20λ	72320	19	67m	5.4×10^{-5}	$2.1 \cdot 10^{-5}$

Table 2: Scattering by an ogive.

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